P5 Science Drivers: Theory

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DOE Exascale Requirements Review (HEP)

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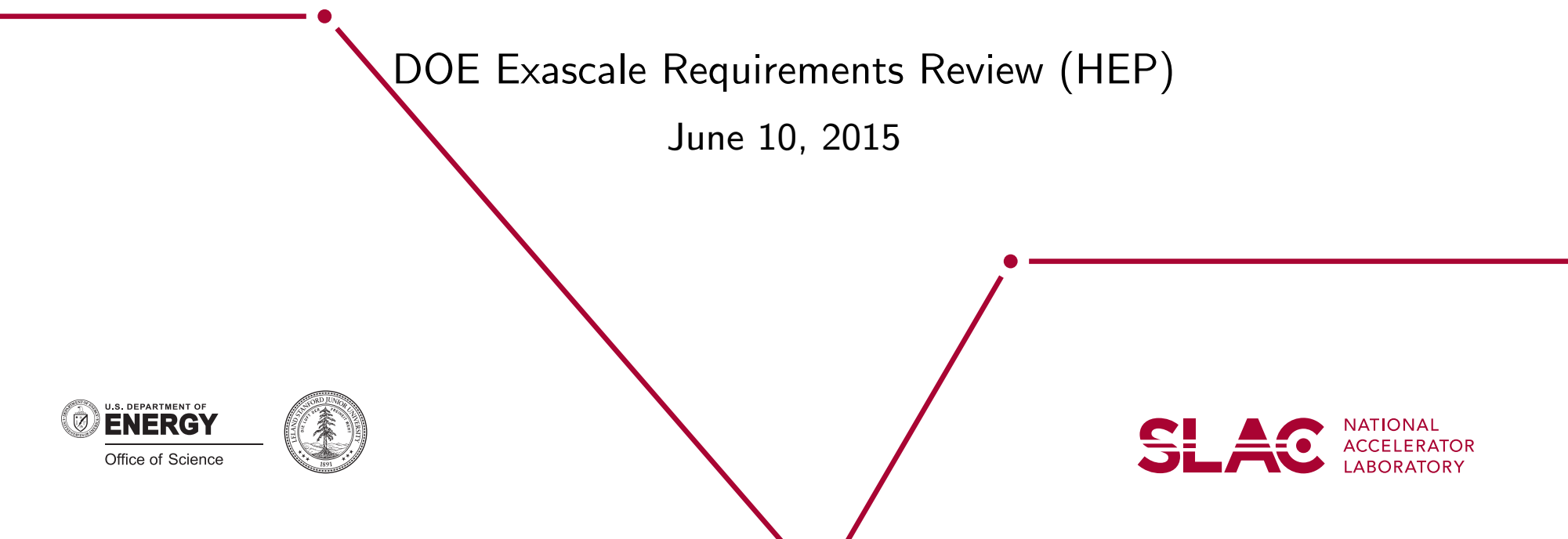

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P5 recommendations

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[http://www.usparticlephysics.org/p5]

From the summary:

- Specific investments in particle accelerator, instrumentation, and computing research and development are required to support the program and to ensure the long-term productivity of the field.

From the report:

- Computing cuts across all activities in particle physics, and these activities spur innovation in computing. The field played leading roles in developing and using high-throughput and distributed/grid computing, online [..] data processing, high-performance computing, high-performance networking, large-scale data storage, large-scale data management and analysis, and the World Wide Web [..]

  Theory computations will continue to increase in importance, as higher fidelity modeling will be required to understand the data.

Traditional HPC: Lattice QCD

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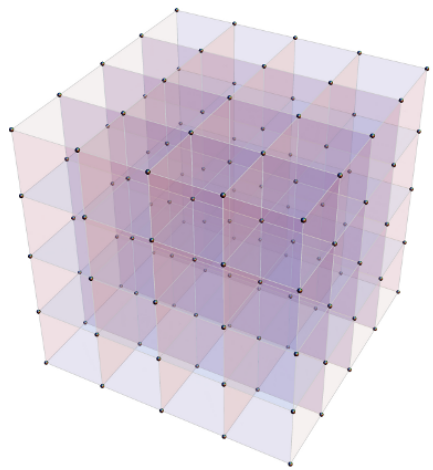
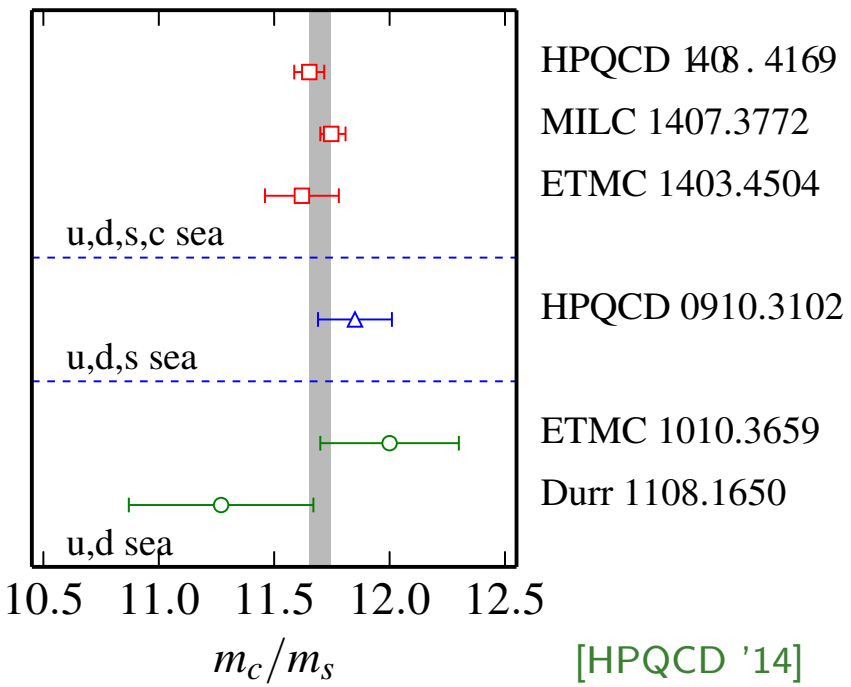
- LQCD is only means to extract SM parameters depending on non-perturbative dynamics of QCD
- Ab-initio calculation in discrete space-time with lattice spacings down to ~ 0.06 fm in $144^3 \times 288$ hypercube
- Systematic errors from continuum extrapolation and chiral extrapolation, the latter lately reduced and soon to be eliminated



Interplay with experiment

- Observables include masses, hadron decay properties and basic Standard Model parameters
- Direct interpretation of BaBar, CLEO, CDF, DØ, Belle, LHCb, BESIII and Belle II experimental data
- Most precise determination of strong coupling from LQCD, needed in search for new physics through Higgs-boson decays at ATLAS & CMS



[HPQCD '14]

- Uncertainty reduction in theory predictions for muon $g-2$ may come from LQCD $\rightarrow$ would directly impact FNAL experiment

Non-tradtitional HPC: Perturbative QCD

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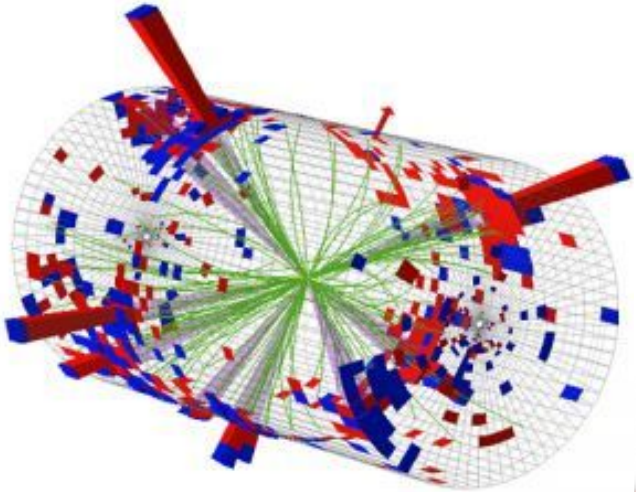
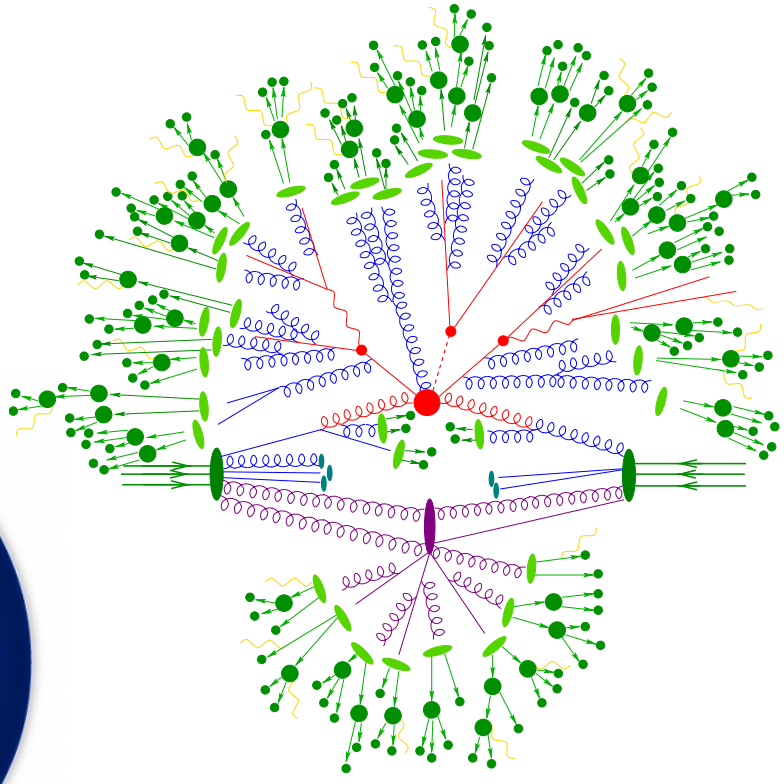
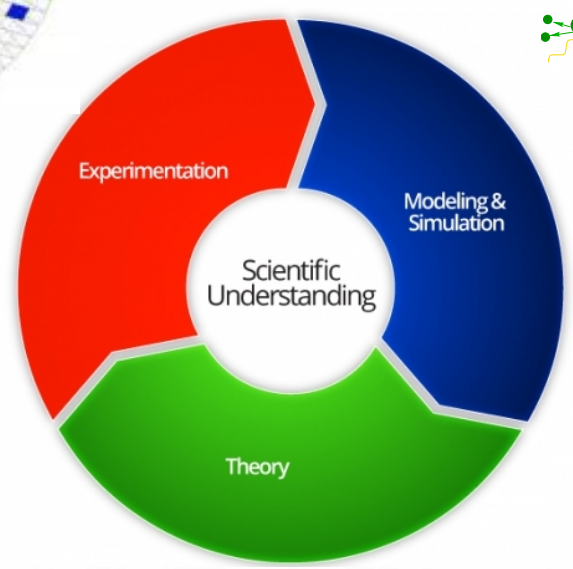
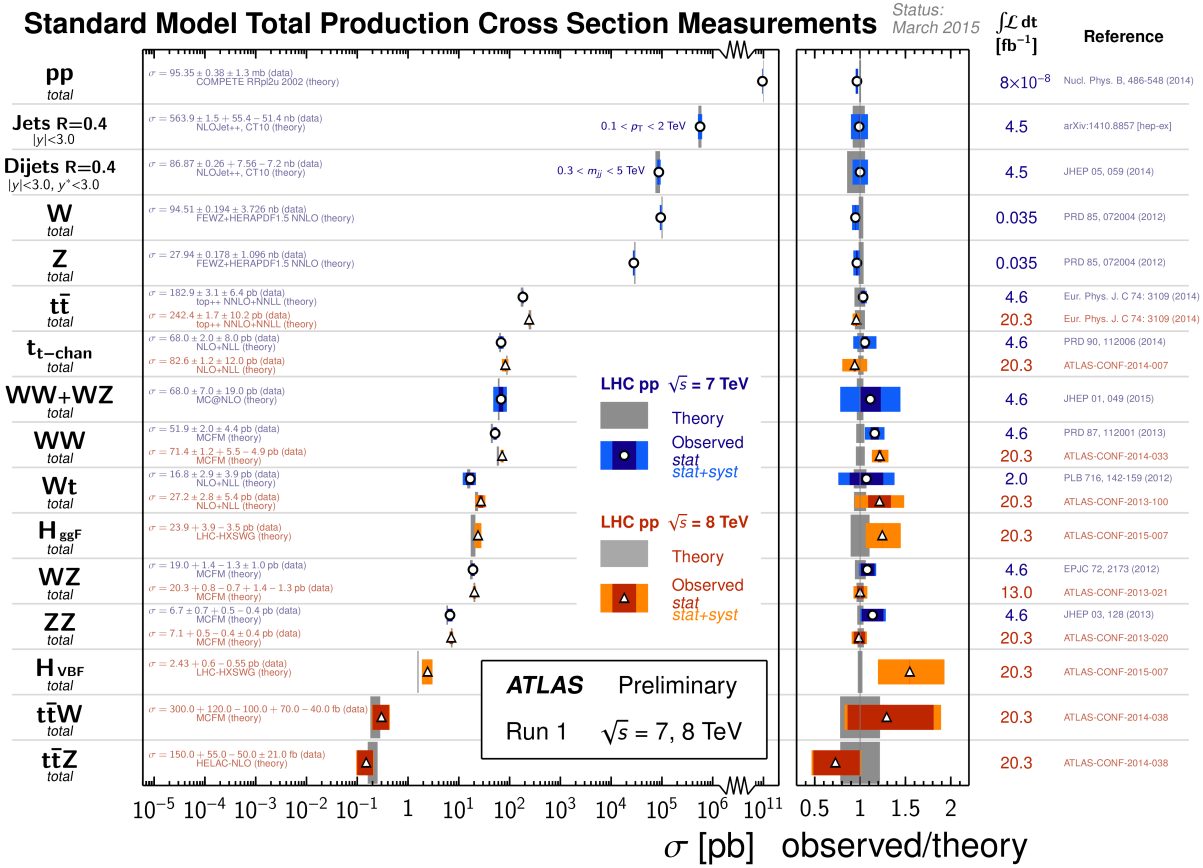


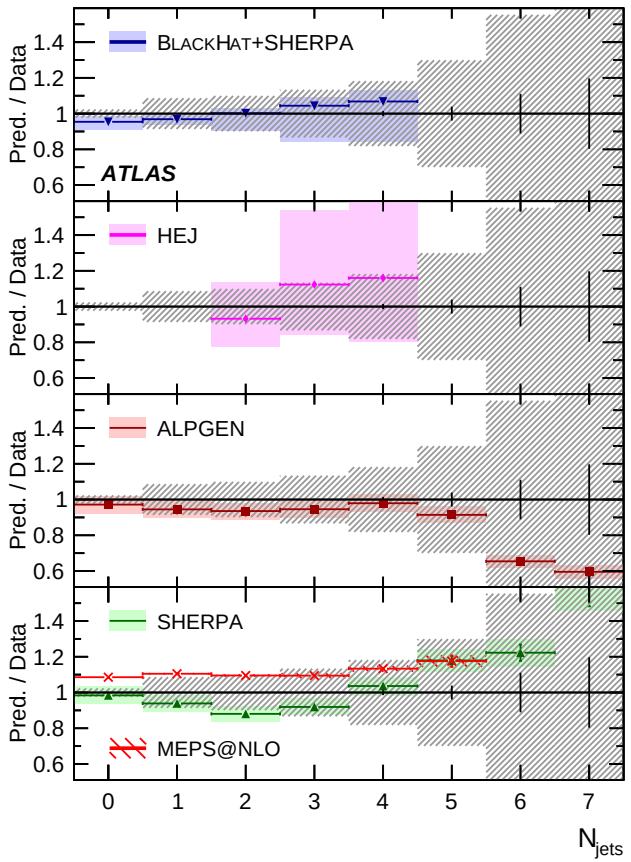




$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c.$$

Interplay with experiment

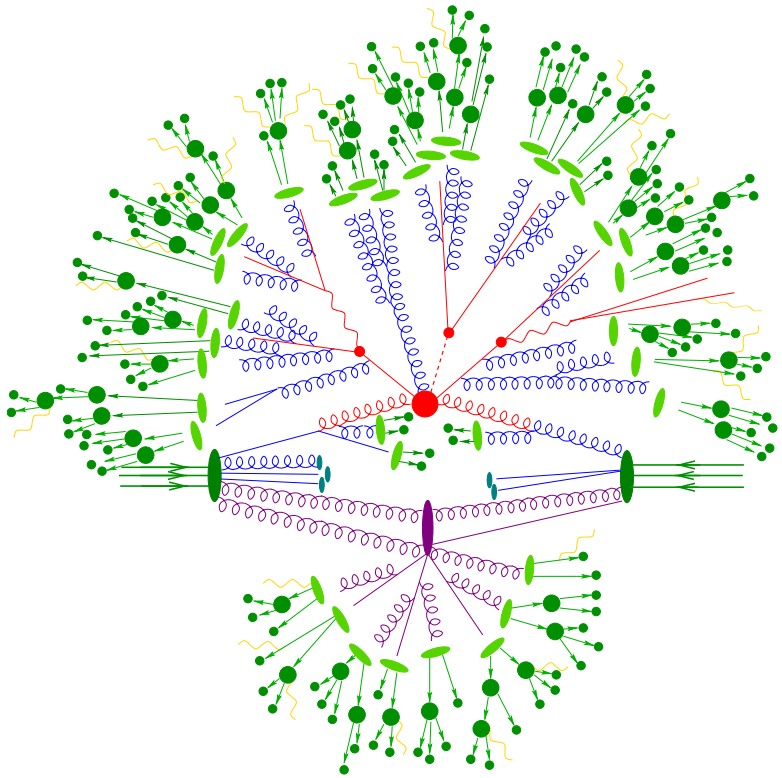




- Both inclusive and fully differential results needed to scrutinize SM
- Particle-level predictions mandatory for direct comparison and unfolding

Aspects of the theory

- Perturbative regime
  - Hard processes
  - Radiative corrections
- Non-perturbative regime
  - Hadronization
  - Particle decays



Divide et Impera

- Quantity of interest: Total interaction rate
- Convolution of short & long distance physics

$$\sigma_{p_1 p_2 \to X} = \sum_{i,j \in \{q,g\}} \int \mathrm{d}x_1 \mathrm{d}x_2 \underbrace{f_{p_1,i}(x_1, \mu_F^2) f_{p_2,j}(x_2, \mu_F^2)}_{\text{long distance}} \underbrace{\hat{\sigma}_{ij \to X}(x_1 x_2, \mu_F^2)}_{\text{short distance}}$$

pQCD Toolkit inventory

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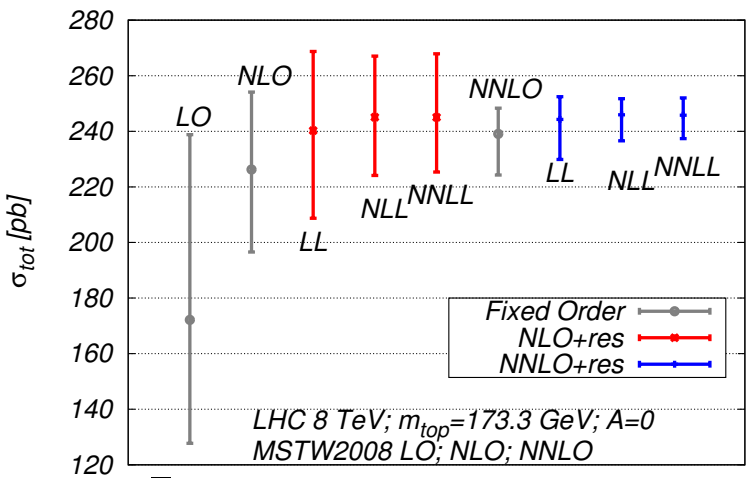
Current state of development

- Parton shower Monte Carlo (Herwig,Pythia,Sherpa,...)
- Automated NLO calculations (BlackHat,GoSam,Helac,MadLoop,MadGolem,NJet,OpenLoops,...)
- Matching to parton shower (aMC@NLO,Herwig,POWHEG Box,Sherpa,...)
- Merging of NLO calculations (aMC@NLO,Helac,Pythia,Sherpa,...)

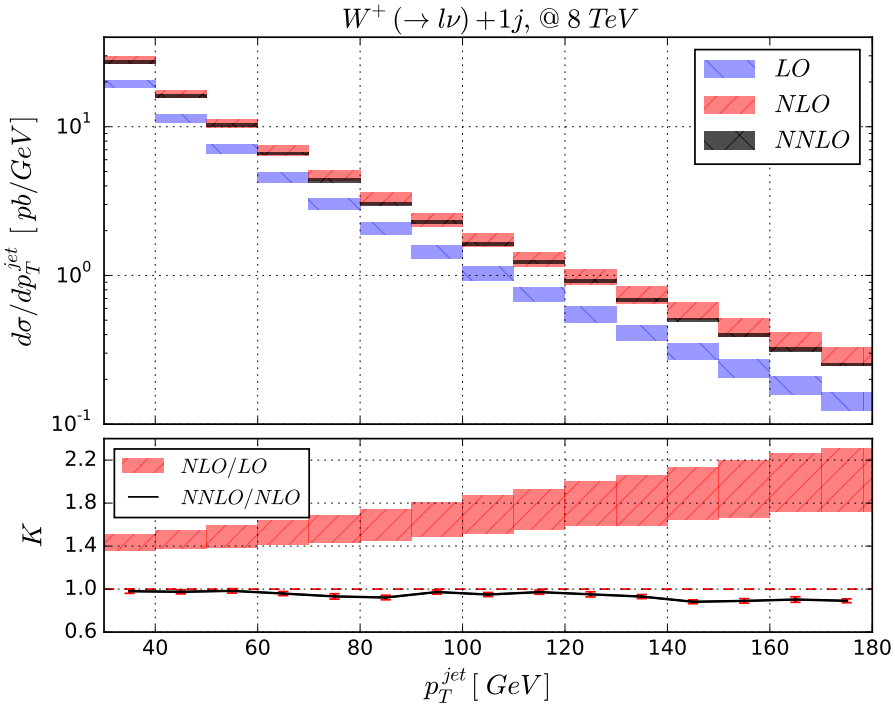
Cutting edge technology & future directions

- Inclusive NNNLO (gg→H)
- Differential NNLO (V/H(+jet),$\gamma\gamma$,VV,...)
- NNLO+N^{x}LL resummation (gg→H,$t\bar{t}$,...)
- NNLO+parton shower (W,Z,gg→H)



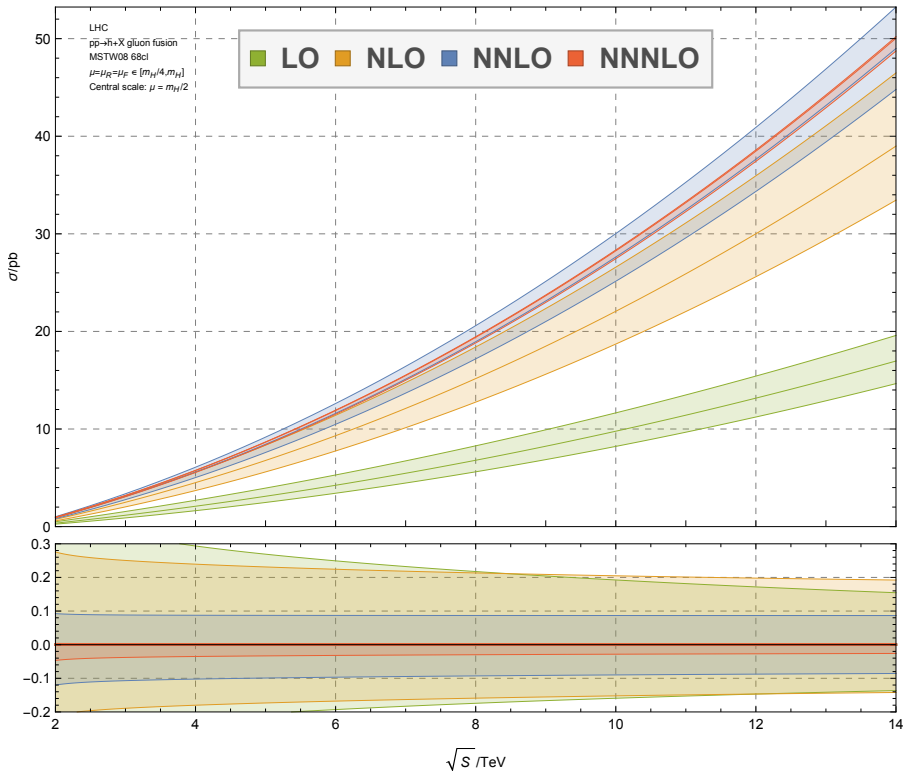
$t\bar{t}$ cross section [Czakon et al.]

Ultra-high precision calculations



[Boughezal,Focke,Liu,Petriello '15]

- New method for regularizing divergences (jettiness subtraction)
- Calculation performed using hybrid MPI+OpenMP approach



[Anastasiou,Duhr,Dulat,Herzog,Mistlberger '15]

- First complete N^{3}LO calculation at a hadron collider
- Total scale variation 3%, reducing theory uncertainty by factor 3

HPC usage projections from Snowmass 2013

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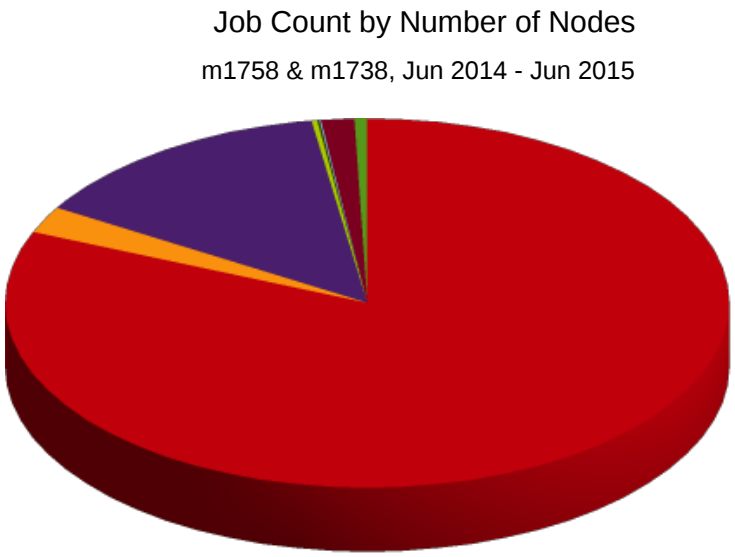
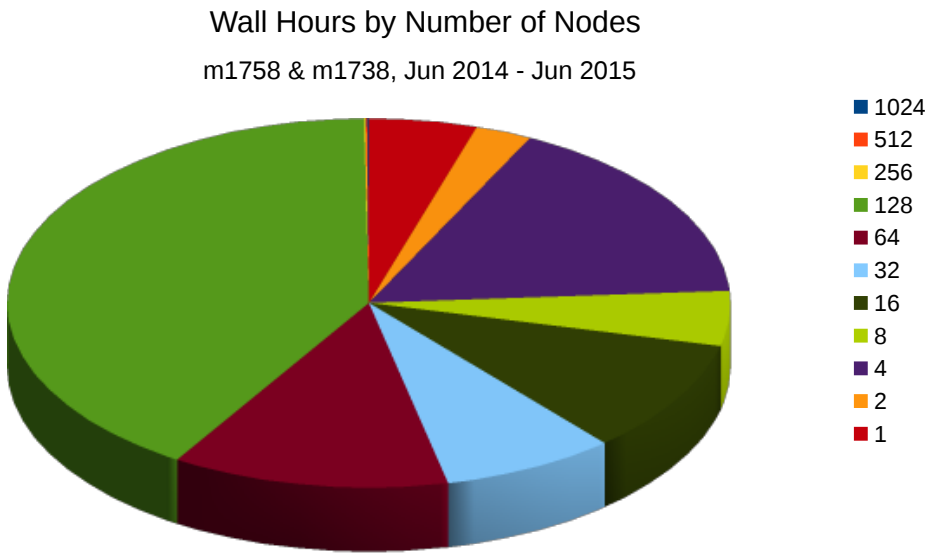
Type of calculation	CPU hours per project	projects per year
NLO parton level	300,000	10-12
Matrix Element Method	200,000	3-5
NNLO parton level	250,000	5-6
Precision event generation	200,000	3
Exclusive jet cross sections	300,000	1-2
Parton Distributions	50,000	5-6
MSSM phenomenology	500,000	10
BSM constraints	150,000	2
Model building	100,000	1-2

- Projected total of $\geq$6M CPUh for pQCD and $\geq$5.45M CPUh for BSM
- Prone to rapid changes depending on theory and technology developments

Actual HPC usage

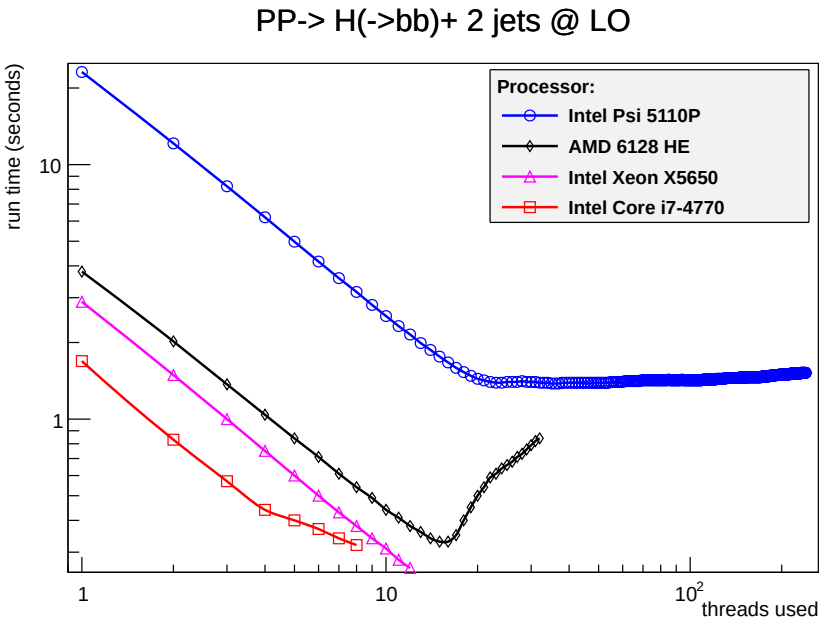


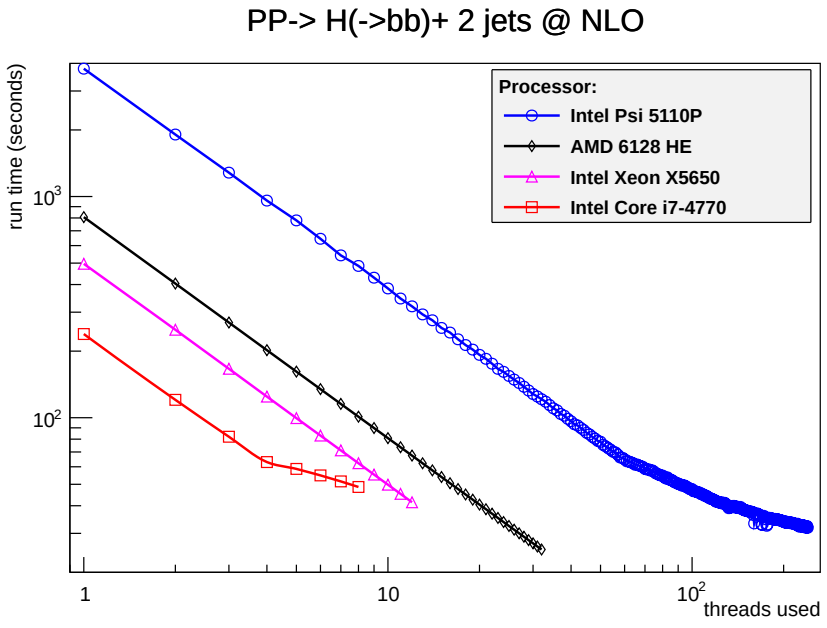


- NERSC usage during past year ∼6.07M CPUh (pQCD only)
- Still at small-scale, but large potential for growth

- 7 publications in 2014, 3 in 2015 (as of Jun 8)
- First (full) calculation of W/H+jet at NNLO arXiv:1504.02131, arXiv:1505.03893
- First NNLO+PS matched simulation for Drell-Yan arXiv:1405.3607

Technology development





- MCFM generator has been a workhorse in NLO calculations for years
- Recently thread- (OpenMP) and MPI-parallelized arXiv:1503.06182
- Used for jettiness subtraction at NNLO arXiv:1505.03893 and arXiv:1504.02131

Summary

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- Theory computing includes traditional and non-tradtional cases
- Lattice QCD has larger needs and well-developed technology
- Perturbative QCD is exploiting a large potential for growth
- BSM phenomenology still to join at larger scale (LBNL only so far)
- Small investments on computing can yield large returns on theory side (example pQCD NNLO W/Z+jet, computed at NERSC)